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Journal of Approximation Theory 146 (2007) 157–173

JOURNAL OF
Approximation
Theory

www.elsevier.com/locate/jat

Asymptotic Gauss–Jacobi quadrature error estimation for Schwarz–Christoffel integrals

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Received 5 April 2006; accepted 20 October 2006

Communicated by Borislav Bojanov

Available online 31 December 2006

Abstract

Numerical conformal mapping packages based on the Schwarz–Christoffel formula have been in existence for a number of years. Various authors, for good reasons of practical efficiency, have chosen to use composite n -point Gauss–Jacobi rules for the estimation of the Schwarz–Christoffel path integrals. These implementations rely on an ad hoc, but experimentally well-founded, heuristic for selecting the spacing of the integration end-points relative to the position of the nearby integrand singularities. In the present paper we derive an explicitly computable estimate, asymptotic as $n \rightarrow \infty$, for the relevant Gauss–Jacobi quadrature error. A numerical example illustrates the potential accuracy of the estimate even at low values of n . It is apparent that the error estimate will allow the adaptive construction of composite rules in a manner that is more efficient than has been possible hitherto.

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PACS: 30C30; 30E15; 41A55; 41A60

Keywords: Gauss–Jacobi quadrature; Asymptotic error estimation; Schwarz–Christoffel formula

1. Introduction

Let w_1, w_2, \dots, w_N be a sequence of N points, each of which lies on the unit circle in the complex plane, and let $\lambda_1, \lambda_2, \dots, \lambda_N$ be an associated sequence of real numbers satisfying

$$-1 \leq \lambda_k < 1, \quad k = 1, \dots, N \quad (1)$$

subject to

$$\sum_{k=1}^N \lambda_k = 2. \quad (2)$$

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The Schwarz–Christoffel integral

$$S[a, b] := \int_a^b \prod_{k=1}^N \left(1 - \frac{z}{w_k}\right)^{-\lambda_k} dz, \quad |a| \leq 1, \quad |b| \leq 1 \quad (3)$$

is the main component in the well-known Schwarz–Christoffel formula for mapping the unit disk conformally onto a N -sided bounded polygon, where w_k is mapped onto the k th vertex of the polygon and $\lambda_k \pi$ is the exterior angle turned through at this vertex. The integration path in (3) is always assumed to be the line segment from a to b , which we denote by $[a, b]$. The integral $S[a, b]$ cannot normally be evaluated analytically and hence it must be estimated numerically. However, the practical issue is not how to estimate $S[a, b]$ accurately, since this may be achieved by a variety of methods including the use of general purpose packages such as Quadpack [9]; rather, the issue is how to estimate $S[a, b]$ efficiently, subject always to reasonable expectations of accuracy. The need for efficiency arises from the fact that, in practical mapping calculations, $S[a, b]$ may need to be computed many thousands of times for different end-points a, b ; see, for example, Driscoll and Trefethen [3, §3.2] for a recent overview of the Schwarz–Christoffel quadrature problem.

If either of the end-points a, b coincides with one of the pre-vertices $\{w_k\}_{k=1}^N$ then the integrand has an algebraic branch point singularity at that end-point. The integrand can have no other singularities on the line of integration, although, depending on the precise location of the points $\{w_k\}_{k=1}^N$, there can be numerous branch point singularities in the vicinity of the integration path. Such integrand singularities are exactly modelled by the classical Jacobi weight function and hence the associated Gauss–Jacobi quadrature scheme is a most natural choice of quadrature method. However, in practice it is essential to employ this scheme in composite form with subinterval end-points selected adaptively so as to reflect the distribution of nearby singularities. A early algorithm for the heuristic implementation of such a scheme is due to Trefethen [10]. This algorithm was incorporated into the Fortran package SCPACK, see Trefethen [11], and subsequently into the MATLAB Toolbox of Driscoll [2]. This same adaptive composite Gauss–Jacobi strategy was also used by Driscoll and Vavasis [4] and, for the case of a modified Schwarz–Christoffel integral, by Howell and Trefethen [8]. The majority of these authors have experimented with alternative quadrature schemes but have all selected Trefethen’s original composite Gauss–Jacobi algorithm because of its inherent efficiency, this despite the fact that the scheme has no in-built quadrature error indicator. This lack of a quadrature error indicator is largely mitigated by the fact that the associated conformal map has its own a posteriori error checks.

The purpose of the present paper is to derive an estimate for the quadrature error when the appropriate Gauss–Jacobi rule is used to approximate $S[a, b]$. More specifically, let $G_n[a, b]$ denote the n -point Gauss–Jacobi quadrature rule estimate for $S[a, b]$ with error

$$E_n[a, b] := S[a, b] - G_n[a, b]. \quad (4)$$

Our main purpose is to derive an explicit directly computable estimate, say $\tilde{E}_n[a, b]$, for $E_n[a, b]$ that is valid asymptotically as $n \rightarrow \infty$. After various preliminaries in Sections 2 and 3 the main result is established in Section 4, where the expression for $\tilde{E}_n[a, b]$ appears in Theorem 3. In Section 5, we present a numerical example. In case the reader should think that the asymptotic regime $n \rightarrow \infty$ may not be practically relevant, this example illustrates that the asymptotic estimate appears to be remarkably accurate even for relatively small single digit values of n .

2. Notational preliminaries

Throughout the paper we use a, b in a generic way to denote integration interval end-points; these may be the end-points for an initial integral or they may define a subinterval used as part of a composite estimate of the initial integral. The possible appearance of end-point singularities in the integrand depends on whether or not a or b coincides with a pre-vertex. In order to have a notation that handles the various cases, we introduce the sets

$$\begin{aligned}\mathcal{P} &:= \{w_1, w_2, \dots, w_N\}, & \text{the set of pre-vertices,} \\ \mathcal{I} &:= \mathcal{P} \cap \{a, b\}, & \text{the set of integration limits that are also pre-vertices,} \\ \mathcal{R} &:= \mathcal{P} \setminus \mathcal{I}, & \text{the remaining set of pre-vertices,}\end{aligned}$$

together with the function $\lambda : \mathbb{C} \mapsto \{\lambda_1, \lambda_2, \dots, \lambda_N\}$ defined by

$$\lambda(w) := \begin{cases} \lambda_k & \text{if } w = w_k, \\ 0 & \text{otherwise.} \end{cases}$$

Remark 1. In practice, in the implementations of the authors mentioned above, it is never required to estimate $S[a, b]$ for the case $\mathcal{I} \equiv \{a, b\}$. This is because the initial interval $[a, b]$ is always subdivided. In this case, one never has to deal with more than $1 + N$ distinct weight functions and the associated standardized n -point quadrature rule weights and nodes can be computed once and for all and stored for later use. Without such an automatic initial subdivision one may need to consider up to $1 + N(N + 1)/2$ different weight functions, a considerable and practically unnecessary overhead. However, as far as the theory is concerned, we continue to allow the case $\mathcal{I} \equiv \{a, b\}$.

In order to make use of standard asymptotic results, it is convenient to change to the standard integration interval $[-1, 1]$. For this purpose, we introduce the linear function ℓ defined by

$$\ell(t) := c + ht, \tag{5}$$

where $c := (a + b)/2$ is the mid-point of the integration interval and $h := (b - a)/2$ is its complex half-length, so that ℓ maps $[-1, 1]$ onto $[a, b]$. Let the pre-images of the sets $\mathcal{P}, \mathcal{I}, \mathcal{R}$ under ℓ be

$$\mathcal{P}^* := \ell^{-1}(\mathcal{P}), \quad \mathcal{I}^* := \ell^{-1}(\mathcal{I}), \quad \mathcal{R}^* := \ell^{-1}(\mathcal{R}),$$

and also introduce the function

$$\lambda^* := \lambda \circ \ell. \tag{6}$$

Hence, writing the Schwarz–Christoffel integrand as

$$s(z) := \prod_{w \in \mathcal{P}} \left(1 - \frac{z}{w}\right)^{-\lambda(w)}, \tag{7}$$

invoking the change of variable $z = \ell(t)$, setting $w = \ell(u)$, noting the identity

$$1 - \frac{z}{w} = \left(1 - \frac{c}{w}\right) \left(1 - \frac{t}{u}\right) \tag{8}$$

and using the fact that $\mathcal{P}^* \equiv \mathcal{I}^* \cup \mathcal{R}^*$, we see that (3) can be written as

$$S[a, b] = hs(c) \int_{-1}^1 (1 - t)^\alpha (1 + t)^\beta f(t) dt, \tag{9}$$

where the Jacobi indices α, β are defined implicitly by the requirement

$$(1-t)^\alpha(1+t)^\beta \equiv \prod_{u \in \mathcal{I}^*} \left(1 - \frac{t}{u}\right)^{-\lambda^*(u)} \quad (10)$$

and

$$f(t) := \prod_{u \in \mathcal{R}^*} \left(1 - \frac{t}{u}\right)^{-\lambda^*(u)}. \quad (11)$$

In interpreting (10) note that there are only four possibilities for the set \mathcal{I}^* , namely $\{-1, 1\}$, $\{-1\}$, $\{1\}$ or \emptyset , so that the indices α, β are uniquely defined by (10). We also note for later reference that constraints (1) and (2) may be written as

$$-1 \leq \lambda^*(u) < 1, \quad u \in \mathcal{P}^* \quad (12)$$

and

$$\sum_{u \in \mathcal{P}^*} \lambda^*(u) = \sum_{u \in \mathcal{R}^*} \lambda^*(u) + \sum_{u \in \mathcal{I}^*} \lambda^*(u) = 2. \quad (13)$$

Hence, from (10) we see that the Jacobi indices satisfy

$$\alpha + \beta = - \sum_{u \in \mathcal{I}^*} \lambda^*(u) = \sum_{u \in \mathcal{R}^*} \lambda^*(u) - 2. \quad (14)$$

At this point it is appropriate to identify more precisely the various Gauss–Jacobi quadrature estimates and associated errors that are the central topics of our discussion. Thus, let

$$G_n^* := \sum_{k=1}^n \mu_k f(t_k)$$

denote the Gauss–Jacobi n -point quadrature estimate for the integral appearing in (9), where $\{\mu_k\}$ and $\{t_k\}$ are the weights and abscissae of the n -point Gaussian quadrature rule associated with the Jacobi weight function $(1-t)^\alpha(1+t)^\beta$. Denote the corresponding quadrature error by

$$E_n^* := \int_{-1}^1 (1-t)^\alpha(1+t)^\beta f(t) dt - G_n^*. \quad (15)$$

It is clear, from (9), that the n -point Gauss–Jacobi estimate for $S[a, b]$ is

$$G_n[a, b] = hs(c)G_n^*$$

and hence that

$$E_n[a, b] = hs(c)E_n^*. \quad (16)$$

3. Branch cut selection

The quadrature error analysis of the next section is primarily concerned with estimating the error E_n^* of (15). This analysis requires that the domain of definition of the integrand f of (11)

be extended to the whole, suitably cut, complex plane. The principal branch cut for the typical fractional power appearing in (11) is the radial line B_u , $u \in \mathcal{R}^*$, defined by

$$B_u := \{t \in \mathbb{C} : t = (1+x)u, x > 0\}.$$

However, any other branch cut which starts at $u \notin [-1, 1]$ and goes out to ∞ without crossing the real line segment $[-1, 1]$ will define a fractional power of $(1-t/u)$ that agrees with the principal value for $t \in [-1, 1]$; we may describe such a branch cut as being computationally equivalent to B_u . It turns out to be most convenient for the subsequent analysis, see Remark 4 below, to use computationally equivalent hyperbolic branch cuts H_u defined by

$$H_u := \{t \in \mathbb{C} : t = \cosh(\cosh^{-1}(u) + x), x > 0\},$$

where the above branch of \cosh^{-1} is defined on $\mathbb{C} \setminus [-1, 1]$ and satisfies

$$\Re(\cosh^{-1}(u)) > 0, \quad -\pi < \Im(\cosh^{-1}(u)) \leq \pi. \quad (17)$$

Thus, in extending the definition of the typical fractional power of (11) to the whole cut plane we assume that

$$\left(1 - \frac{t}{u}\right)^{-\lambda^*(u)} := \exp\left(-\lambda^*(u) \log\left(1 - \frac{t}{u}\right)\right),$$

where \log denotes the logarithm function with branch cut H_u defined by

$$\log\left(1 - \frac{t}{u}\right) := \int_0^t \frac{d\tau}{\tau - u}, \quad \tau \notin H_u. \quad (18)$$

Now suppose that ϕ is any function which has a finite jump discontinuity across the cut H_u but is otherwise analytic in the vicinity of H_u . If $t \in H_u$ then

$$t' := \sinh(\cosh^{-1}(u) + x), \quad x > 0$$

is tangential to H_u and defines the positive direction along H_u ; this positive direction is always outwards, away from u towards ∞ . Let us define the jump in the value of ϕ across the cut H_u at the point t as

$$[\phi(t)]|_{H_u} := \lim_{\varepsilon \rightarrow 0} (\phi(t + i\varepsilon t') - \phi(t - i\varepsilon t')), \quad \varepsilon > 0, t \in H_u. \quad (19)$$

Lemma 1. *If $t \in H_u$ then*

$$\left[\left(1 - \frac{t}{u}\right)^{-\lambda^*(u)}\right]|_{H_u} = 2i \sin(\pi\lambda^*(u)) \left(\frac{t}{u} - 1\right)^{-\lambda^*(u)}, \quad (20)$$

where the fractional power on the right above takes its principal value.

Proof. In order to have a clear understanding of the relationship between the fractional powers involved, it is probably best to revert to first principles. Thus let Log denote the principal branch of the logarithm defined by

$$\text{Log}\left(\frac{t}{u} - 1\right) := \int_1^{\frac{t}{u}-1} \frac{d\zeta}{\zeta}, \quad \zeta \notin (-\infty, 0).$$

Changing the variable of integration to $\tau := u(\zeta + 1)$ gives

$$\operatorname{Log} \left(\frac{t}{u} - 1 \right) = \int_{2u}^t \frac{d\tau}{\tau - u}, \quad \tau \notin B_u^c, \quad (21)$$

where the branch cut B_u^c is complementary to B_u and is defined by

$$B_u^c := \{t \in \mathbb{C} : t = (1 - x)u, \ x > 0\}.$$

Observe that B_u^c has no points in common with H_u and hence $\operatorname{Log}(\frac{t}{u} - 1)$ is analytic at $t \in H_u$. Now consider the simple closed contour $C \cup L \cup (-C^+)$, where C is the semi-circle with center u , radius $|u|$, traversed from 0 to $2u$ in the anti-clockwise direction, L is the line segment from $2u$ to $t \in H_u$ and C^+ is any simple curve from 0 to $t \in H_u$, not intersecting $C \cup L$, meeting H_u orthogonally at t so as to contain the limit points $t + i\epsilon t'$ for sufficiently small ϵ and such that $u \in \operatorname{int}(C \cup L \cup (-C^+))$; see Fig. 1 for an illustration of the case where u lies in the first quadrant with $|2u| < |t|$. Cauchy's formula gives

$$\int_C \frac{d\tau}{\tau - u} + \int_L \frac{d\tau}{\tau - u} - \int_{C^+} \frac{d\tau}{\tau - u} = 2\pi i.$$

The first integral above may be evaluated directly to give

$$\int_C \frac{d\tau}{\tau - u} = \pi i$$

and the second is a special case of (21) so that

$$\int_L \frac{d\tau}{\tau - u} = \operatorname{Log} \left(\frac{t}{u} - 1 \right).$$

Thus, using definition (18) and the defining properties of C^+ it follows from the above results that

$$\lim_{\epsilon \rightarrow 0} \log \left(1 - \frac{t + i\epsilon t'}{u} \right) = \int_{C^+} \frac{d\tau}{\tau - u} = \operatorname{Log} \left(\frac{t}{u} - 1 \right) - \pi i. \quad (22)$$

In a similar manner consider the simple closed contour $C \cup L \cup (-C^-)$, where C^- is any simple curve from 0 to $t \in H_u$, not intersecting $C \cup L$, meeting H_u orthogonally at t so as to contain the limit points $t - i\epsilon t'$ for sufficiently small ϵ and such that $u \notin \operatorname{int}(C \cup L \cup (-C^-))$; see Fig. 1. In this case Cauchy's theorem gives

$$\int_C \frac{d\tau}{\tau - u} + \int_L \frac{d\tau}{\tau - u} - \int_{C^-} \frac{d\tau}{\tau - u} = 0$$

and we deduce that

$$\lim_{\epsilon \rightarrow 0} \log \left(1 - \frac{t - i\epsilon t'}{u} \right) = \int_{C^-} \frac{d\tau}{\tau - u} = \operatorname{Log} \left(\frac{t}{u} - 1 \right) + \pi i. \quad (23)$$

Thus, applying definition (19) and using (22), (23) we obtain

$$\left[\left(1 - \frac{t}{u} \right)^{-\lambda^*(u)} \right] \Big|_{H_u} = \lim_{\epsilon \rightarrow 0} \left\{ \begin{array}{l} \exp \left(-\lambda^*(u) \log \left(1 - \frac{t + i\epsilon t'}{u} \right) \right) \\ - \exp \left(-\lambda^*(u) \log \left(1 - \frac{t - i\epsilon t'}{u} \right) \right) \end{array} \right\}$$

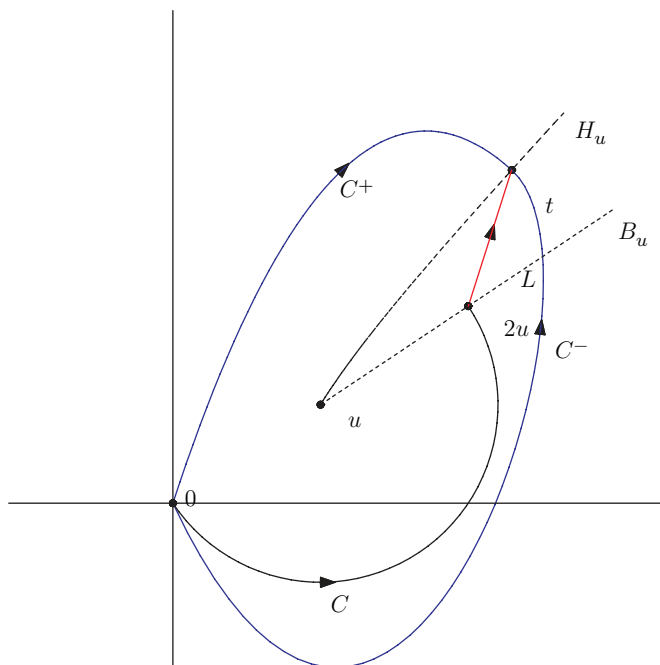


Fig. 1. The construction of C^+ and C^- for u in the first quadrant and $|2u| < |t|$.

$$\begin{aligned}
 &= \exp\left(-\lambda^*(u)\left(\operatorname{Log}\left(\frac{t}{u}-1\right)-i\pi\right)\right) \\
 &\quad - \exp\left(-\lambda^*(u)\left(\operatorname{Log}\left(\frac{t}{u}-1\right)+i\pi\right)\right) \\
 &= \left(\frac{t}{u}-1\right)^{-\lambda^*(u)} (\exp(i\pi\lambda^*(u)) - \exp(-i\pi\lambda^*(u))),
 \end{aligned}$$

which completes the proof since the final fractional power is defined in terms of the principal branch of the logarithm function. \square

4. Asymptotic analysis

Following Donaldson and Elliott [1, Theorem 1], the error E_n^* of (15) can be expressed in the form

$$E_n^* = \frac{1}{2\pi i} \int_C \eta^{(\alpha, \beta)}(t) dt, \quad (24)$$

where

$$\eta^{(\alpha, \beta)}(t) := \frac{\Pi_n^{(\alpha, \beta)}(t)}{P_n^{(\alpha, \beta)}(t)} f(t), \quad (25)$$

$P_n^{(\alpha, \beta)}$ is the Jacobi polynomial of degree n and $\Pi_n^{(\alpha, \beta)}$ denotes the Jacobi function of the second kind defined by

$$\Pi_n^{(\alpha, \beta)}(t) := \int_{-1}^1 \frac{(1-x)^\alpha (1+x)^\beta P_n^{(\alpha, \beta)}(x)}{t-x} dx. \quad (26)$$

Note that $\Pi_n^{(\alpha, \beta)}$ is analytic in the cut plane $\mathbb{C} \setminus [-1, 1]$. The integration path C in (24) may be any simple closed curve, traversed in the anticlockwise direction, which encircles the segment $[-1, 1]$ but does not cross the branch cuts H_u , $u \in \mathcal{R}^*$. It is an elementary task to prove that if $u, v \in \mathcal{R}^*$ and $u \neq v$ then $H_u \cap H_v \equiv \emptyset$ and we omit the details. A natural choice for C is as follows. First, surround each point $u \in \mathcal{R}^*$ by a circle C_u with center u and suitably small radius δ so that C_u does not intersect the line segment $[-1, 1]$. Then form an outer circle C_0 , centered at 0 with suitably large radius ρ , so that each C_u lies in the interior of C_0 , and link C_0 to each C_u , $u \in \mathcal{R}^*$, by a cross-cut L_u which runs along the branch cut H_u . The path C then consists of C_0 traversed in the anti-clockwise direction and, for each $u \in \mathcal{R}^*$, the two edges of the cross-cut L_u together with C_u traversed in the clockwise direction. With the above definition for C it follows that

$$\int_C \eta^{(\alpha, \beta)}(t) dt = \int_{C_0} \eta^{(\alpha, \beta)}(t) dt + \sum_{u \in \mathcal{R}^*} \left\{ \int_{L_u} [\eta^{(\alpha, \beta)}(t)]|_{H_u} dt - \int_{C_u} \eta^{(\alpha, \beta)}(t) dt \right\}, \quad (27)$$

where $[\cdot]|_{H_u}$ is the jump across the cut H_u as defined by (19).

Theorem 1. *With notation as above,*

$$E_n^* = \sum_{u \in \mathcal{R}^*} \frac{\sin(\pi \lambda^*(u))}{\pi} \int_{H_u} \frac{\Pi_n^{(\alpha, \beta)}(t) g(t, u)}{P_n^{(\alpha, \beta)}(t)} \left(\frac{t}{u} - 1 \right)^{-\lambda^*(u)} dt, \quad (28)$$

where

$$g(t, u) := \prod_{v \in \mathcal{R}^* \setminus \{u\}} \left(1 - \frac{t}{v} \right)^{-\lambda^*(v)}, \quad u \in \mathcal{R}^*. \quad (29)$$

Proof. The idea of the proof is simply to show that the contour integrals around C_0 and C_u , $u \in \mathcal{R}^*$, in (27) tend to zero as $\rho \rightarrow \infty$ and $\delta \rightarrow 0$, respectively. The result then follows from (24).

It is clear from (11), (25) and the above definition of g that for any $u \in \mathcal{R}^*$

$$\eta^{(\alpha, \beta)}(t) := \frac{\Pi_n^{(\alpha, \beta)}(t) g(t, u)}{P_n^{(\alpha, \beta)}(t)} \left(1 - \frac{t}{u} \right)^{-\lambda^*(u)}. \quad (30)$$

It is also clear from (29) that the only points t at which $g(t, u)$ may fail to be analytic are precisely those points which lie on the branch cuts H_v for $v \in \mathcal{R}^* \setminus \{u\}$. Thus, $g(t, u)$ is analytic at $t \in H_u$ and therefore at all points t sufficiently close to H_u . This has two consequences.

In the first place, since $\Pi_n^{(\alpha, \beta)}(t)/P_n^{(\alpha, \beta)}(t)$ is analytic on $\mathbb{C} \setminus [-1, 1]$, it follows from (30) and (20) that

$$[\eta^{(\alpha, \beta)}(t)]\Big|_{H_u} = 2i \sin(\pi \lambda^*(u)) \frac{\Pi_n^{(\alpha, \beta)}(t)g(t, u)}{P_n^{(\alpha, \beta)}(t)} \left(\frac{t}{u} - 1\right)^{-\lambda^*(u)}. \quad (31)$$

Secondly, the maximum principle for analytic functions ensures that the quantity

$$M(\delta) := \max_{t \in C_u} \left| \frac{\Pi_n^{(\alpha, \beta)}(t)g(t, u)}{P_n^{(\alpha, \beta)}(t)} \right| \quad (32)$$

ultimately decreases monotonically as $\delta \rightarrow 0$. Thus, making use of (30) and introducing the parameterization $t = u + \delta e^{i\theta}$, $\theta_0 \leq \theta \leq \theta_0 + 2\pi$, for the circle C_u we see that

$$\left| \int_{C_u} \eta^{(\alpha, \beta)}(t) dt \right| \leq 2\pi \delta^{1-\lambda^*(u)} |u|^{\lambda^*(u)} M(\delta)$$

which, in view of (12), leads to the conclusion

$$\lim_{\delta \rightarrow 0} \int_{C_u} \eta^{(\alpha, \beta)}(t) dt = 0. \quad (33)$$

It remains to prove that the first integral on the right of (27) tends to zero as $\rho \rightarrow \infty$. At this point several details of the analysis follow those given in [7] and are therefore only outlined here. Substituting (25) and (26) in the relevant integral from (27), interchanging the order of integration, making use of the absolutely convergent power series expansion of $(x - t)^{-1}$ for large $\rho = |t|$ and $x \in [-1, 1]$ we lead to the result

$$\begin{aligned} \int_{C_0} \eta^{(\alpha, \beta)}(t) dt &= \sum_{k=n}^{\infty} \left\{ \left(\int_{-1}^1 (1-x)^{\alpha} (1+x)^{\beta} P_n^{(\alpha, \beta)}(x) x^k dx \right) \right. \\ &\quad \times \left. \left(\int_{C_0} \frac{f(t)}{P_n^{(\alpha, \beta)}(t) t^{k+1}} dt \right) \right\}, \end{aligned} \quad (34)$$

where use has also been made of the orthogonality properties of the Jacobi polynomials. The rational function $t^n/P_n^{(\alpha, \beta)}(t)$ is analytic on $\mathbb{C} \setminus [-1, 1]$ and hence the maximum principle implies that

$$\max_{t \in C_0} \left| \frac{t^n}{P_n^{(\alpha, \beta)}(t)} \right| \leq \max_{|t|=1} \left| \frac{1}{P_n^{(\alpha, \beta)}(t)} \right| =: L_n^{(\alpha, \beta)}. \quad (35)$$

From (11) we see that

$$f(t) = \prod_{u \in \mathcal{R}^*} t^{-\lambda^*(u)} \prod_{u \in \mathcal{R}^*} \left(\frac{1}{t} - \frac{1}{u} \right)^{-\lambda^*(u)}.$$

Hence, using (14) it follows that

$$\max_{t \in C_0} |f(t)| \leq \frac{M(\rho)}{\rho^{2+\alpha+\beta}}, \quad (36)$$

where now we have re-defined M as

$$M(\rho) := \max_{t \in C_0} \prod_{u \in \mathcal{R}^*} \left| \frac{1}{t} - \frac{1}{u} \right|^{-\lambda^*(u)},$$

with

$$\lim_{\rho \rightarrow \infty} M(\rho) = \prod_{u \in \mathcal{R}^*} |u|^{\lambda^*(u)}. \quad (37)$$

Also, as demonstrated in [7],

$$\left| \int_{-1}^1 (1-x)^\alpha (1+x)^\beta P_n^{(\alpha, \beta)}(x) x^k dx \right| \leq M_n^{(\alpha, \beta)}, \quad k \geq n \geq 1, \quad (38)$$

where

$$M_n^{(\alpha, \beta)} := \max_{-1 \leq x \leq 1} \left(\frac{(1-x)^{\alpha+1} (1+x)^{\beta+1} |P_{n-1}^{(\alpha+1, \beta+1)}(x)|}{n} \right).$$

Hence, using (35), (36) and (38) in (34), we see that

$$\left| \int_{C_0} \eta^{(\alpha, \beta)}(t) dt \right| \leq \frac{M(\rho) M_n^{(\alpha, \beta)} L_n^{(\alpha, \beta)}}{\rho^{2+\alpha+\beta}} \sum_{k=n}^{\infty} \int_{C_0} \frac{|dt|}{|t|^{k+1+n}} = \frac{M(\rho) M_n^{(\alpha, \beta)} L_n^{(\alpha, \beta)}}{\rho^{2+\alpha+\beta+n} (1-\rho^{-1})}.$$

Thus, since $\alpha + \beta + 2 > 0$ and in view of (37) it follows from the previous result that, for any $n \geq 1$, there holds

$$\lim_{\rho \rightarrow \infty} \left| \int_{C_0} \eta^{(\alpha, \beta)}(t) dt \right| = 0. \quad (39)$$

Finally, substituting (31) into (27), allowing $\rho \rightarrow \infty$ and $\delta \rightarrow 0$, using the results (33), (39) and noting that in the limit, L_u approaches the full semi-infinite branch cut H_u , the result stated in the theorem follows. \square

Donaldson and Elliott [1] have described a general and elegant approach to the estimation of quadrature errors via the use of asymptotic estimates for $P_n^{(\alpha, \beta)}$ and $\Pi_n^{(\alpha, \beta)}$ as $n \rightarrow \infty$. We take this same approach, and start by recalling a number of established results.

The following three lemmas are proved, respectively, in [7], Henrici [6, §11.5] and Elliott [5].

Lemma 2. *Given any $u \in \mathbb{C} \setminus [-1, 1]$, let ϕ be any function for which the associated function Φ defined by*

$$\Phi(x) := \sinh(\zeta + x) \phi \circ \cosh(\zeta + x), \quad \zeta := \cosh^{-1}(u), \quad 0 \leq x < \infty,$$

has a well-defined Laplace transform

$$\mathcal{L}\Phi(s) := \int_0^\infty e^{-sx} \Phi(x) dx.$$

Then

$$\int_{H_u} \frac{\phi(t)}{(t + \sqrt{t^2 - 1})^n} dt = \frac{\mathcal{L}\Phi(n)}{(u + \sqrt{u^2 - 1})^n}.$$

Lemma 3 (Watson–Doetsch). *If Φ has an asymptotic power series*

$$\Phi(x) \sim x^\gamma \sum_{k=0}^{\infty} \Phi_k x^{k\lambda} = x^\gamma \Phi_0 + \dots$$

as $x \rightarrow 0$, $x > 0$, then $\mathcal{L}\Phi$ has the asymptotic power series

$$\mathcal{L}\Phi(n) \sim \frac{1}{n^{\gamma+1}} \sum_{k=0}^{\infty} \frac{\Phi_k \Gamma(\gamma+1+k\lambda)}{n^{k\lambda}} = \frac{\Phi_0 \Gamma(\gamma+1)}{n^{\gamma+1}} + \dots$$

as $n \rightarrow \infty$.

Lemma 4. *If t is bounded away from $[-1, 1]$ then the leading term in the asymptotic expansion of $\Pi_n^{(\alpha, \beta)}(t)/P_n^{(\alpha, \beta)}(t)$ as $n \rightarrow \infty$ is given by*

$$\frac{\Pi_n^{(\alpha, \beta)}(t)}{P_n^{(\alpha, \beta)}(t)} \sim \frac{N_n^{(\alpha, \beta)}(t-1)^\alpha(1+t)^\beta}{(t+\sqrt{t^2-1})^{2n+\alpha+\beta+1}},$$

where

$$N_n^{(\alpha, \beta)} := 2^{4n+2\alpha+2\beta+2} \frac{\Gamma(n+1)\Gamma(n+\alpha+1)\Gamma(n+\beta+1)\Gamma(n+\alpha+\beta+1)}{\Gamma(2n+\alpha+\beta+2)\Gamma(2n+\alpha+\beta+1)}.$$

Remark 2. In Lemma 4 the principal branch is used for the fractional powers; typically this means that $|\arg(t \pm 1)| < \pi$. The expression $\sqrt{t^2-1}$ should be interpreted as $(t-1)^{\frac{1}{2}}(t+1)^{\frac{1}{2}}$, thus ensuring that $|t+\sqrt{t^2-1}| > 1$. This treatment should also be applied to the same expression arising in Lemma 2.

Remark 3. The inverse function \cosh^{-1} appearing in Lemma 2 is that previously defined by (17).

Remark 4. Throughout this section prior to Lemma 2, the hyperbolic branch cut H_u , wherever it occurs, could be replaced by the principal cut B_u without altering any of the results, including the statement of Theorem 1. The results stated in Lemma 2 depend critically on the cut being parameterized by a hyperbolic function. At this point, therefore, the use of the branch cut H_u allows an easy connection to be made with Laplace transform theory and the Watson–Doetsch Lemma 3.

Theorem 2. *The expression*

$$\tilde{E}_n^* := \frac{N_n^{(\alpha, \beta)}}{\pi} \sum_{u \in \mathcal{R}^*} \left(\frac{(u-1)^{\alpha+\frac{1}{2}-\frac{\lambda^*(u)}{2}}(u+1)^{\beta+\frac{1}{2}-\frac{\lambda^*(u)}{2}} u^{\lambda^*(u)}}{(u+\sqrt{u^2-1})^{2n+\alpha+\beta+1}} \times \frac{\sin(\pi\lambda^*(u))g(u, u)\Gamma(1-\lambda^*(u))}{(2n+\alpha+\beta+1)^{1-\lambda^*(u)}} \right)$$

defines a computable estimate for E_n^ which is valid asymptotically as $n \rightarrow \infty$.*

Proof. Substituting the leading term of the asymptotic expansion from Lemma 4 into (28) and making use of the result of Lemma 2 we see that the leading term in the asymptotic expansion of

E_n^* may be written as

$$E_n^* \sim \frac{N_n^{(\alpha, \beta)}}{\pi} \sum_{u \in \mathcal{R}^*} \frac{\sin(\pi \lambda^*(u)) \mathcal{L}\Phi(2n + \alpha + \beta + 1)}{(u + \sqrt{u^2 - 1})^{2n + \alpha + \beta + 1}}, \quad (40)$$

where

$$\phi(x) := (x - 1)^\alpha (x + 1)^\beta g(x, u) \left(\frac{x}{u} - 1\right)^{-\lambda^*(u)}$$

and, as in the statement of Lemma 2,

$$\Phi(x) := \sinh(\zeta + x) \phi \circ \cosh(\zeta + x), \quad \zeta := \cosh^{-1}(u), \quad u \in \mathcal{R}^*.$$

Assuming all limits were to exist, then it would follow from the above definitions, bearing in mind $u \notin [-1, 1]$, that

$$\begin{aligned} \lim_{x \rightarrow 0} \Phi(x) &= (u^2 - 1)^{\frac{1}{2}} \lim_{x \rightarrow 0} \phi \circ \cosh(\zeta + x) \\ &= (u^2 - 1)^{\frac{1}{2}} (u - 1)^\alpha (u + 1)^\beta g(u, u) \lim_{x \rightarrow 0} \left(\frac{\cosh(\zeta + x)}{u} - 1 \right)^{-\lambda^*(u)}. \end{aligned}$$

However, it is clear that

$$\frac{\cosh(\zeta + x)}{u} - 1 = x \frac{(u^2 - 1)^{\frac{1}{2}}}{u} + O(x^2)$$

so that, as $x \rightarrow 0$, we conclude that

$$\Phi(x) \sim \Phi_0 x^{-\lambda^*(u)} + \dots$$

with

$$\Phi_0 := (u - 1)^{\alpha + \frac{1}{2} - \frac{\lambda^*(u)}{2}} (u + 1)^{\beta + \frac{1}{2} - \frac{\lambda^*(u)}{2}} u^{\lambda^*(u)} g(u, u).$$

Using these results in conjunction with Lemma 3 we may use (2) to obtain the dominant term in the asymptotic expansion of E_n^* as $n \rightarrow \infty$; this gives the estimate \tilde{E}_n^* stated in the theorem. \square

By using Theorem 2 together with (16) we may derive an estimate for the quadrature error $E_n[a, b]$. This is the main result of the paper and is presented as Theorem 3 below. In preparation for this we introduce the function G defined by

$$G(w) := \frac{\sin(\pi \lambda(w)) \Gamma(1 - \lambda(w))}{w^{2n}} \prod_{v \in \mathcal{P} \setminus \{w\}} \left(1 - \frac{w}{v}\right)^{-\lambda(v)}. \quad (41)$$

Clearly, $G(w)$ is independent of the integration end-points a, b and may be computed once and for all for each $w \in \mathcal{P}$.

Theorem 3. *With notation as previously defined, the expression*

$$\tilde{E}_n[a, b] := \sum_{w \in \mathcal{R}} T_n(w), \quad (42)$$

where

$$T_n(w) := \frac{h^{2n+1} N_n^{(\alpha, \beta)}(w) G(w)}{\pi(2n + \alpha + \beta + 1)^{1-\lambda(w)} \prod_{v \in \mathcal{I}} \left(1 - \frac{c}{v}\right)^{-\lambda(v)} \prod_{v \in \mathcal{I}} \left(1 - \frac{w}{v}\right)^{\lambda(v)}} \\ \times \frac{(1-b/w)^{\alpha+\frac{1}{2}-\frac{\lambda(w)}{2}} (1-a/w)^{\beta+\frac{1}{2}-\frac{\lambda(w)}{2}}}{(1-c/w + \sqrt{1-a/w} \sqrt{1-b/w})^{2n+\alpha+\beta+1}} \quad (43)$$

defines a computable estimate for $E_n[a, b]$ which is valid asymptotically as $n \rightarrow \infty$.

Proof. In view of (16) our asymptotic estimate for $E_n[a, b]$ is defined as

$$\tilde{E}_n[a, b] := h s(c) \tilde{E}_n^*, \quad (44)$$

where \tilde{E}_n^* is defined in Theorem 2. It simply remains to reorganize this expression by undoing the changes of variable introduced in Section 2. Specifically, for each $u \in \mathcal{R}^*$ we have $w = \ell(u)$, $w \in \mathcal{R}$, where ℓ is defined by (5), so that

$$u - 1 = \frac{w}{h} \left(1 - \frac{b}{w}\right), \quad u + 1 = \frac{w}{h} \left(1 - \frac{a}{w}\right), \quad u = \frac{w}{h} \left(1 - \frac{c}{w}\right).$$

Making use of the above relationships and recalling from (6) that $\lambda^*(u) = \lambda \circ \ell(u) = \lambda(w)$, it follows that

$$\frac{(u-1)^{\alpha+\frac{1}{2}-\frac{\lambda^*(u)}{2}} (u+1)^{\beta+\frac{1}{2}-\frac{\lambda^*(u)}{2}} u^{\lambda^*(u)}}{(u + \sqrt{u^2 - 1})^{2n+\alpha+\beta+1}} \\ = \left(\frac{h}{w}\right)^{2n} \frac{(1-b/w)^{\alpha+\frac{1}{2}-\frac{\lambda(w)}{2}} (1-a/w)^{\beta+\frac{1}{2}-\frac{\lambda(w)}{2}} (1-c/w)^{\lambda(w)}}{(1-c/w + \sqrt{1-a/w} \sqrt{1-b/w})^{2n+\alpha+\beta+1}}. \quad (45)$$

Similarly, for $u \in \mathcal{R}^*$ and $w = \ell(u) \in \mathcal{R}$, we may use definition (29) together with a factorization of the type (8) to deduce that

$$g(u, u) = \prod_{v \in \mathcal{R} \setminus \{w\}} \left(1 - \frac{w}{v}\right)^{-\lambda(v)} \prod_{v \in \mathcal{R} \setminus \{w\}} \left(1 - \frac{c}{v}\right)^{\lambda(v)}. \quad (46)$$

Also, since $w \in \mathcal{R}$ implies that $\mathcal{P} \setminus \{w\} \equiv (\mathcal{R} \setminus \{w\}) \cup \mathcal{I}$, we see from (41) that

$$G(w) = \frac{\sin(\pi \lambda(w)) \Gamma(1 - \lambda(w))}{w^{2n}} \prod_{v \in \mathcal{R} \setminus \{w\}} \left(1 - \frac{w}{v}\right)^{-\lambda(v)} \prod_{v \in \mathcal{I}} \left(1 - \frac{w}{v}\right)^{-\lambda(v)} \quad (47)$$

and, since $\mathcal{P} \equiv (\mathcal{R} \setminus \{w\}) \cup \mathcal{I} \cup \{w\}$, it follows from (7) that

$$s(c) = \left(1 - \frac{c}{w}\right)^{-\lambda(w)} \prod_{v \in \mathcal{R} \setminus \{w\}} \left(1 - \frac{c}{v}\right)^{-\lambda(v)} \prod_{v \in \mathcal{I}} \left(1 - \frac{c}{v}\right)^{-\lambda(v)}. \quad (48)$$

Elimination of the product over the set $\mathcal{R} \setminus \{w\}$ between (46) and (47) allows us to write $g(u, u)$, $u \in \mathcal{R}^*$, in terms of $G(w)$, $w = \ell(u) \in \mathcal{R}$, and hence using (48) it follows that

$$s(c) \sin(\pi \lambda^*(u)) g(u, u) \Gamma(1 - \lambda^*(u)) \\ = w^{2n} G(w) \left(1 - \frac{c}{w}\right)^{-\lambda(w)} \prod_{v \in \mathcal{I}} \left(\left(1 - \frac{w}{v}\right)^{\lambda(v)} \left(1 - \frac{c}{v}\right)^{-\lambda(v)} \right). \quad (49)$$

Finally, substituting the expression for \tilde{E}_n^* as defined in Theorem 2 into (44) and making use of (45) and (49), the result stated in the theorem follows.

5. Numerical example

In this section, we consider a simple but realistic example with $N = 8$ pre-vertices defined by

$$w_k := \frac{\rho + e^{i\theta_k}}{1 + \rho e^{i\theta_k}}, \quad \theta_k := \frac{\pi i(k-1)}{4}, \quad k = 1, 2, \dots, 8, \quad 0 \leq \rho < 1 \quad (50)$$

and exterior angle parameters

$$\lambda_k := \frac{1}{4}, \quad k = 1, 2, \dots, 8.$$

The above data arises in the case where the unit disc is conformally mapped onto a regular octagon, such that the point ρ on the positive real axis is mapped onto the center of the octagon. For all choices of ρ we have

$$w_1 = 1, \quad w_5 = -1, \quad w_{10-k} = \bar{w}_k, \quad k = 2, 3, 4.$$

As $\rho \rightarrow 1$ the pre-vertices, with the exception of w_5 , crowd around the point $w_1 = 1$ making for a more difficult quadrature problem.

We consider the specific case

$$\rho = \frac{2\sqrt{2}}{3}$$

so that (50) gives

$$w_2 = \sqrt{2} \frac{41+i}{58}, \quad w_3 = \frac{12\sqrt{2}+i}{17}, \quad w_4 = \sqrt{2} \frac{7+i}{10}.$$

These pre-vertices are moderately crowded around $w_1 = 1$; see Fig. 2.

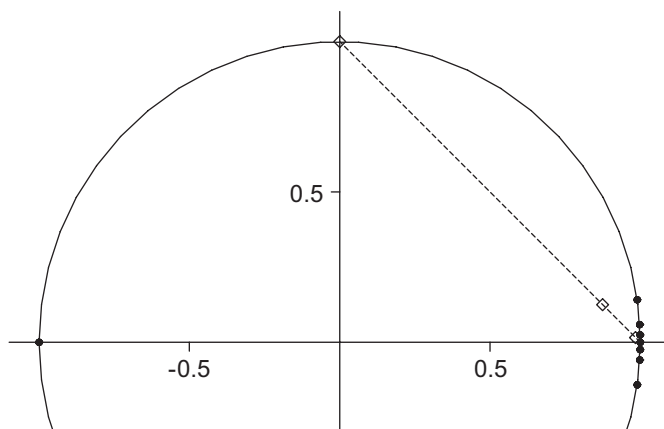


Fig. 2. Singular points at pre-vertices \bullet and integration end-points \diamond .

Table 1
Quadpack estimates for $S[1, \gamma(s)]$

s	$Q[1, \gamma(s)]$
$\frac{1}{64}$	$-3.854450022438 + 2.267635483595i$
$\frac{1}{8}$	$-11.66965351854 + 2.192637400823i$
1	$-14.66931612456 + 0.6171079499072i$

Table 2
Comparison of asymptotic and quadpack error estimates

n	$ \tilde{E}_n[1, \gamma(s)] $ (asymptotic)			$ \hat{E}_n[1, \gamma(s)] $ (quadpack)		
	$s = \frac{1}{64}$	$s = \frac{1}{8}$	$s = 1$	$s = \frac{1}{64}$	$s = \frac{1}{8}$	$s = 1$
4	1.5×10^{-5}	1.3×10^{-1}	2.2	1.6×10^{-5}	1.4×10^{-1}	2.8
8	4.1×10^{-10}	9.5×10^{-3}	6.1×10^{-1}	4.2×10^{-10}	9.7×10^{-3}	6.8×10^{-1}
16	4.5×10^{-19}	4.9×10^{-5}	5.8×10^{-2}	†	5.0×10^{-5}	5.9×10^{-2}
32	8.7×10^{-37}	2.2×10^{-9}	1.8×10^{-3}	†	2.2×10^{-9}	1.7×10^{-3}

We then consider the Gauss–Jacobi estimates for the Schwarz–Christoffel integral $S[1, \gamma(s)]$ where

$$\gamma(s) := 1 + s(i - 1).$$

In this case, the pre-vertex w_1 is an integration limit, so that

$$\mathcal{I} = \{w_1\},$$

and the Jacobi indices associated with $S[1, \gamma(s)]$ are

$$\alpha = 0, \quad \beta = -\frac{1}{4}.$$

We compute the error estimate $\tilde{E}_n[1, \gamma(s)]$ for the cases $s = 1, \frac{1}{8}, \frac{1}{64}$ and $n = 4, 8, 16, 32$. This is compared with the reliable independent error estimate

$$\hat{E}_n[1, \gamma(s)] := Q[1, \gamma(s)] - G_n[1, \gamma(s)],$$

where $Q[a, b]$ denotes the Quadpack approximation for $S[a, b]$ using the routine DQDAWS with absolute and relative error tolerances set at 10^{-13} ; see [9]. The various Quadpack quadrature estimates are given in Table 1. The magnitudes of $\tilde{E}_n[1, \gamma(s)]$ and $\hat{E}_n[1, \gamma(s)]$ are compared in Table 2, where † indicates that the estimate $\hat{E}_n[1, \gamma(\frac{1}{64})]$ has reached the level of machine precision, about 10^{-16} in this case.

It is clear that as the length of an integration interval is reduced the pre-vertices become relatively more distant from the interval and the strengths of their singularities become weaker. This is illustrated in Table 3, which shows the magnitude of each term in the sum defining $\tilde{E}_n[1, \gamma(s)]$ for the case $n = 8$ and $s = \frac{1}{64}, 1$; the pre-vertices are ordered by the size of their respective contributions to $\tilde{E}_8[1, \gamma(1)]$. In both cases, but especially for the shorter interval, the value of $|\tilde{E}_n[1, \gamma(s)]|$ arises almost entirely from the term contributed by the nearest singularity at w_2 .

Table 3

Magnitudes of errors arising from individual pre-vertices

Pre-vertex	Magnitude of contribution to $\tilde{E}_8[1, \gamma(s)]$	
	$s = \frac{1}{64}$	$s = 1$
w_2	4.07×10^{-10}	5.66×10^{-1}
w_3	4.43×10^{-17}	2.14×10^{-1}
w_8	9.54×10^{-14}	5.29×10^{-2}
w_4	4.22×10^{-24}	3.16×10^{-2}
w_7	6.87×10^{-19}	5.45×10^{-3}
w_6	7.18×10^{-25}	1.09×10^{-4}
w_5	1.50×10^{-44}	6.81×10^{-13}

6. Conclusion

We have derived a computable estimate $\tilde{E}_n[a, b]$ which converges asymptotically as $n \rightarrow \infty$ to the true Gauss–Jacobi quadrature error $E_n[a, b]$ of (4). The numerical example of Section 5 demonstrates the potential practical accuracy of this estimate, even for relatively small values of n . We suggest that the main practical use of this estimate should be as the quadrature error indicator in the construction of adaptive composite Gauss–Jacobi rules for the Schwarz–Christoffel integral.

The estimate $\tilde{E}_n[a, b]$ is derived only for the case of Schwarz–Christoffel integrals on a disc with a linear integration path. The asymptotic theory and general approach outlined above will readily extend to alternative integration paths on the disc, to Schwarz–Christoffel integrals defined on a half-plane and to the modified Schwarz–Christoffel integrals arising in the infinite strip mappings considered by Howell and Trefethen [8]. However, and this is clearly a weakness of the present approach, the analytic details will need to be re-worked for these different cases.

We finally note that the elegant and general quadrature error theory of Donaldson and Elliott [1] has received relatively little practical consideration. One reason for this is that in order to apply Donaldson and Elliott’s theory one needs fairly complete information about the distribution of integrand singularities over the whole complex plane. However, for the quadratures of classical potential theory, complex analysis and elastostatics, where the kernels are explicitly known but analytically intractable, such singularity information is often available. Therefore, in these applications, if the practical demand is to perform quadratures as efficiently as possible, then the extra analysis required by the Donaldson and Elliott theory may well yield significant dividends in terms of producing efficient and acceptably accurate error estimates.

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